

Pimelic acid, 4-chlorobenzyl octyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-2-3-4-5-6-10-17-26-21(24)11-8-7-9-12-22(25)27-18-19-13-15
InchiKey:	PRLOKJMEVMOPBE-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-242.63	kJ/mol	Joback Method
hf	-777.69	kJ/mol	Joback Method
hfus	56.16	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.237		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	924.43	K	Joback Method
tc	1134.12	K	Joback Method
tf	550.88	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.36	J/molxK	924.43	Joback Method
cpg	1039.76	J/molxK	959.38	Joback Method
cpg	1053.89	J/molxK	994.33	Joback Method
cpg	1066.80	J/molxK	1029.27	Joback Method
cpg	1078.52	J/molxK	1064.22	Joback Method
cpg	1089.07	J/molxK	1099.17	Joback Method
cpg	1098.50	J/molxK	1134.12	Joback Method
dvisc	0.0003880	Paxs	550.88	Joback Method

dvisc	0.0002123	Paxs	613.14	Joback Method
dvisc	0.0001298	Paxs	675.40	Joback Method
dvisc	0.0000862	Paxs	737.65	Joback Method
dvisc	0.0000611	Paxs	799.91	Joback Method
dvisc	0.0000454	Paxs	862.17	Joback Method
dvisc	0.0000352	Paxs	924.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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